

From Electronic Dynamics to Fully Coupled Electronic-Nuclear Dynamics

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Molecular control at the time and length scale of the electron is a grand challenge for science, which may be achieved using ultrashort laser pulses down to the attosecond time scale. In order to understand and predict phenomena arising from the interaction between laser pulses and matter, we are forced to solve the time-dependent Schrödinger equation for both electronic and nuclear degrees of freedom. I will give a brief overview of our recent work on explicitly time-dependent quantum-mechanical methods, both laser-induced electronic dynamics within the Born-Oppenheimer approximation [1-4] and coupled electronic-nuclear dynamics without the Born-Oppenheimer approximation [5]. For the electronic dynamics part, emphasis will be put on the interpretation of time-dependent coupled-cluster theory in terms of autocorrelation functions and stationary-state populations, whereas the non-Born-Oppenheimer part will focus on the important phenomenon of laser-induced molecular alignment.

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[2] H. Kristiansen, Ø. S. Schøyen, S. Kvaal, and T.B. Pedersen, *J. Chem. Phys.* **152**, 071102 (2020)

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[4] H. Kristiansen, B. S. Ofstad, E. Hauge, E. Aurbakken, Ø. S. Schøyen, S. Kvaal, and T. B. Pedersen, *J. Chem. Theory Comput.* in press (2022) [arXiv: 2112.13611]

[5] L. Adamowicz, S. Kvaal, C. Lasser, and T. B. Pedersen, arXiv: 2205.15229